

## *Conference Program*

# ***Excited State Processes in Electronic and Bio Nano-Materials***

August 11-16, 2003  
Los Alamos, New Mexico, USA

*Sponsored by Center for Nonlinear Studies, Theoretical, Chemistry, Materials Science and Technology, and Bioscience Divisions at Los Alamos National Laboratory and supported by the U.S. Department of Energy.*

*Organizers:* Sergei Tretiak, Avadh Saxena, and Richard L. Martin.

*Scientific Advisors:* Alan R. Bishop, Andrew P. Shreve, and Victor I. Klimov

*Location:* Motorola Building, Los Alamos Research Park, Los Alamos, NM

## Monday, August 11

**08:00am – 08:30am**      **Registration**

**08:30am – 08:55am**      **Welcome:** Don Parkin (*CINT Associate Director, MST Division*), Rod Garcia (*Conference Coordinator, CNLS*)

### **Biological Systems and Molecular Aggregates**

*Session chair:*              Todd Martinez (University of Illinois)

**08:55am – 09:40am**      **Paul Champion** (Northeastern University)

*"Exploring low frequency modes in biomolecules using femtosecond coherence spectroscopy"*

**09:40am – 10:25am**      **Alexei Stuchebrukhov** (University of California, Davis)

*"Electron transfer in proteins"*

**10:25am – 10:40am**      **Break**

**10:40am – 11:25am**      **Shigehiko Hayashi** (Kyoto University, Japan)

*"Molecular dynamics simulation of bacteriorhodopsin's photoisomerization using ab initio forces for the excited chromophore"*

**11:25am – 12:10pm**      **Sharon Hammes-Schiffer** (Pennsylvania State University)

*"Proton-coupled electron transfer reactions"*

**12:10pm – 12:35pm**      **Yang Zhao, M-F. Ng, and G. Chen** (University of Hong Kong)

*"Low-lying excited states of light-harvesting system II in purple bacteria"*

**12:35pm – 02:00pm**      **Lunch**

*Session chair:*              Anne Myers Kelley (University of California, Merced)

**02:00pm – 02:45pm**      **Qiang Cui** (University of Wisconsin, Madison)

*"Hybrid QM/MM studies of bioluminescent proteins"*

**02:45pm – 03:30pm**      **GuanHua Chen** (University of Hong Kong, Hong Kong)

*"Optical response and field emission of carbon nanotubes"*

**03:30pm – 03:55pm**      **Verner Kristian Thorsmølle** (LANL)

*"Ultrafast conductivity dynamics in pentacene probed using terahertz time-domain spectroscopy"*

**03:55pm – 04:10pm**      **Break**

**04:10pm – 04:55pm**      **Donal Bradley** (University of Sheffield, UK)

*"Energy transfer and light emission in organic semiconductors"*

**04:55pm – 05:40pm**      **David Beljonne** (Université de Mons, Belgium)

*"Quantum-chemical modeling of charge and energy transfer in supramolecular assemblies"*

**05:40pm – 06:00pm**      **Discussion Panel**

*Moderator:*                  Anne Myers Kelley and Todd Martinez

**06:00pm**                      **Reception**

## Tuesday, August 12

### Biological Systems and Molecular Aggregates

*Session chair:* David Yaron (Carnegie Mellon University)

**08:30am – 09:15am**      **Devens Gust** (Arizona State University)

*“Molecular photovoltaics, switches, and photonic wires based on porphyrins and fullerenes”*

**09:15am – 10:00am**      **Frank Spano** (Temple University)

*“Understanding the photophysical properties of lamellar and herringbone aggregates of conjugated oligomers: excitons, phonons and defects”*

**10:00am – 10:25am**      **Eugene Tsiper** (Rutgers University)

*“Atomic multipole representation of molecular response to external fields”*

**10:25am – 10:40am**      **Break**

**10:40am – 11:25am**      **Vladimir Chernyak** (Corning Inc.)

*“Topological properties of conical intersections in higher-dimensional configuration spaces”*

**11:25am – 12:10pm**      **Robert Austin** (Princeton University)

*“Picosecond conformational dynamics of proteins: proteins are nanomachines in nanotime”*

**12:10pm – 12:35pm**      **Valter Zazubovich**, R. Jankowiak, K. Riley, M. Rätsep and G. J. Small (Iowa State University) *“Dispersive kinetics of primary charge separation in the isolated reaction center of photosystem II studied with spectral hole burning”*

**12:35pm – 02:00pm**      **Lunch**

*Session chair:* Avadh Saxena (LANL)

### Semiconductor Quantum Dots

**02:00pm – 02:45pm**      **David Nesbitt** (University of Colorado)

*“Time dependent power law fluorescence dynamics semiconductor quantum dots”*

**02:45pm – 03:10pm**      **Han Htoon**, J. A. Hollingsworth, A. V. Malko, R. Dickerson, and V. I. Klimov (LANL) *“Zero-to-one dimensional transition and Auger recombination in semiconductor nanorods”*

### Poster Session

*Poster session chair:* Sergei Tretiak (LANL)

**03:10pm – 03:30pm**      **Preparation**

**03:30pm – 06:30pm**      **Poster Session, Reception**

## Wednesday, August 13

### Semiconductor Quantum Dots

*Session chair:* Victor Klimov (LANL)

**08:30am – 09:15am** Arthur Nozik (NREL)

*"Relaxation dynamics and interparticle electron transfer dynamics in photoexcited semiconductor nanocrystals"*

**09:15am – 10:00am** Alexandr Efros (Naval Research Laboratory)

*"General boundary conditions and effect of the surface on the energy spectra of nanocrystals"*

**10:00am – 10:25am** Marc Achermann, M.A. Petruska, J. A. Hollingsworth, and V. I. Klimov, (LANL) *"Exciton-exciton interactions in semiconductor nanocrystals: The effect on lasing and light harvesting performance"*

**10:25am – 10:40am** Break

**10:40am – 11:25am** David Gershoni (Technion, Israel)

*"Semiconductor Quantum dots as sources of correlated multicolor single photons"*

**11:25am – 12:10pm** David Norris (University of Minnesota)

*"In Vivo Imaging of Quantum Dots"*

**12:10pm – 12:35pm** Richard Schaller, M. A. Petruska, S. Jeong, J. A. Hollingsworth and V. I. Klimov, (LANL) *"PbSe quantum dots and quantum rods: From optical gain to polarized emission"*

**12:35pm – 02:00pm** Lunch

*Session chair:* Alexandr Efros (Naval Research Laboratory)

**02:00pm – 02:45pm** Gregory Scholes (University of Toronto)

*"Relating electronic structure to optical response: comparison of conjugated polymers to semiconductor quantum dots"*

**02:45pm – 03:30pm** David Kelley (University of California, Merced)

*"Electronic spectroscopy of GaSe nanoparticles"*

**03:30pm – 03:55pm** Melissa Petruska, A. V. Malko, P. M. Voyles, and V. I. Klimov (LANL)

*"From individual nanocrystals to functional nanocrystal assemblies"*

**03:55pm – 04:10pm** Break

**04:10pm – 04:55pm** Ananth Dodabalapur (University of Texas at Austin)

*"What can we do with organic transistors?"*

**04:55pm – 05:15pm** Discussion Panel

*Moderators:* Victor Klimov and Alexandr Efros

**07:00pm** Banquette

## Thursday, August 14

### Semiconductor Quantum Dots

Session chair: Richard Martin (LANL)

**08:30am – 09:15am** **Todd Krauss** (University of Rochester)

*"Localized charge properties of single semiconductor quantum rods"*

**09:15am – 09:40am** **Vanessa Huxter**, M.R. Salvador, and G.D. Scholes (University of Toronto)

*"Two dimensional photon echo studies of nanocrystalline quantum dots"*

**09:40am – 10:05am** **Brian Wehrenberg** and P. Guyot-Sionnest (University of Chicago)

*"Optical and electrochromic properties of colloidal PbSe nanocrystals"*

**10:05am – 10:20am** **Break**

### Metal Nanoparticles and Complexes

**10:20am – 11:05am** **Thomas Meyer** (LANL)

*"Photoinduced electron and energy transfer in molecular assemblies"*

**11:05am – 11:50am** **James Brozik** (University of New Mexico)

*"Extent of localization in the excited states of platinum acetylenic compounds"*

**11:50am – 12:15pm** **Jiang Jiang** and Louis Brus (Columbia University)

*"Single molecule raman spectroscopy at the junctions of large Ag nanocrystals"*

**12:15pm – 12:40pm** **Alexander Mikhailovsky**, J. Ostrowski, M. Katiyar, and G. Bazan (UCSB) *"Control of radiative processes using surface plasmon resonances in metal nanostructures"*

**12:40pm – 02:00pm** **Lunch**

Session chair: Guillermo Bazan (UCSB)

**02:00pm – 02:45pm** **Neil Greenham** (Cavendish Laboratory, UK)

*"Recombination in polymer heterojunction devices"*

**02:45pm – 03:30pm** **Darryl Smith** (LANL)

*"Electron spin injection from ferromagnetic contacts"*

**03:30pm – 03:45pm** **Break**

### Organic Electronic Materials and Polymers

**03:45pm – 04:30pm** **Joseph Perry** (University of Arizona)

*"Two-Photon properties of conjugated organic molecules and nanocomposites"*

**04:30pm – 04:55pm** **Egbert Zojer**, D. Beljonne, W. Wenseleers, S.J.K. Pond, M. Rumi, M. Halik, S. Barlow, C. Grasso, J.W. Perry, S. Marder, and J.-L. Brédas (University of Arizona)

*"Design of materials with enhanced two-photon absorption properties – influence of ground-state polarization, charge-transfer distance and nature of the conjugated backbone"*

**04:55pm – 05:20pm** **Mariacristina Rumi**, S.J.K. Pond, D. Beljonne, O. Kwon, E. Zojer, M.L. Levin, T.C. Parker, O. Tsutsumi, J.-L. Brédas, S.R. Marder, and J.W. Perry (University of Arizona)

*"Substituent effects on the spectroscopic properties of two-photon absorbing chromophores"*

**05:20pm – 05:45pm** **Artem Masunov** and S. Tretiak (LANL)

*"Prediction of two photon absorption properties for large organic molecules using time-dependent density functional theory"*

**05:45pm – 06:10pm** **Discussion Panel**

Moderators: David Yaron and Guillermo Bazan

## Friday, August 15

### Organic Electronic Materials and Polymers

Session chair: Zeev Valy Vardeny (University of Utah)

**08:30am – 09:15am Takayoshi Kobayashi** (University of Tokyo, Japan)

*"Geometrical relaxation studied by ultrashort pulselaser"*

**09:15am – 10:00am Josef Klafter** (Tel Aviv University, Israel)

*"Fractional kinetics in transport and relaxation"*

**10:00am – 10:25am Andrei Piryatinski, S. Tretiak, A. Saxena, R.L. Martin, and A.R. Bishop** (LANL) *"Non-adiabatic dynamics in electron phonon coupled system"*

**10:25am – 10:40am Break**

**10:40am – 11:25am Alan Bishop** (LANL)

*"Photoexcitation and energy localization in soft electronic matter"*

**11:25am – 12:10pm Christopher Bardeen** (University of Illinois)

*"Picosecond dynamics in nanoscale aggregates of conjugated organic materials"*

**12:10pm – 12:35pm Vladimir Butko** (LANL)

*"Progress in organic single crystal electronics"*

**12:35pm – 02:00pm Lunch**

Session chair: Sumit Mazumdar (University of Arizona)

**02:00pm – 02:45pm Kieron Burke** (Rutgers University)

*"Time-dependent density functional theory for electronic and bio nanomaterials"*

**02:45pm – 03:30pm Gustavo Scuseria** (Rice University)

*"Carbon single-wall nanotubes density of states: comparison of experiment and theory, and the role of defects"*

**03:30pm – 03:55pm Ignacio Franco** and S. Tretiak (University of Toronto)

*"Electron-vibrational dynamics of photoexcited polyfluorenes"*

**03:55pm – 04:10pm Break**

**04:10pm – 04:55pm Anna Krylov** (University of Southern California)

*"Tuning molecular properties by electronic excitations"*

**04:55pm – 05:40pm Filipp Furche** (Universität Karlsruhe, Germany)

*"Exploring excited potential energy surfaces by analytical TDDFT derivative methods"*

**05:40pm – 06:00pm Discussion Panel**

Moderators: Zeev Valy Vardeny and Sumit Mazumdar

## Saturday, August 16

### Organic Electronic Materials and polymers

*Session chair:* Darryl Smith (LANL)

**08:30am – 09:15am** **Martin Kirk** (University of New Mexico)

*"Low-Dimensional materials: new paradigms for molecular bistability"*

**09:15am – 10:00am** **John McKelvey** (McKelvey Computational Chemistry)

*"An efficient scheme for determining light absorption properties"*

**10:00am – 10:25am** **Rudolph Magyar**, E.K.U. Gross, and A. Fleszar (Rutgers University)

*"Exact-exchange density-functional calculations on noble-gas solids"*

**10:25am – 10:40am** **Break**

**10:40am – 11:05am** **Geoff Hutchison** (Northwestern University)

*"Studies on transparent conducting polymers"*

**11:05am – 11:30am** **Oleg Korovyanko**, C.-X. Sheng and Z.V. Vardeny, A. Dalton and R. Baughman (University of Utah) *"Ultrafast electronic relaxation in semiconductor and metallic single walled carbon nanotubes"*

**11:30am – 11:55am** **Reginaldo Rocha**, M.G. Brown, C.H. Londergan, C.P. Kubiak and A.P. Shreve (LANL) *"Probing mixed-valency in molecular charge-transfer systems"*

**11:55am – 12:20pm** **Dmitri Kilin**, Y.V. Pereversev, O.V. Prezhdo (University of Washington)

*"Electron-nuclear correlations for photoinduced dynamics in molecular dimers"*

**12:20pm – 12:45pm** **Paul Day**, K.A. Nguyen and R. Pachter (WPAFB)

*"Theoretical predictions of two-photon absorption in substituted stilbenes: a time-dependent density functional theory study"*

**12:45pm – 01:00pm** **Closing remarks**

## Poster Session

**Tuesday, August 12**

- 1. Darius Abramavicius** and S. Mukamel (University of Rochester)  
*"Disentangling complex multidimensional spectra of excitons using coherent control"*
- 2. Thomas Baker** (JILA and University of Colorado)  
*"Using Visible Light to Generate Silver Nanoparticles"*
- 3. Enrique Batista** (LANL)  
*"Density Functional Study of Organoactinide Complexes"*
- 4. Liu Bin**, G. Bazan, B. Koehler, H. Benmansour, A. Mikhailovsky, and J. Hong (UCSB)  
*"Two Photon Absorbing Dyes"*
- 5. Luke Campbell** (University of Rochester)  
*"TBA"*
- 6. Joshua Coe** (University of Illinois)  
*"Nonadiabatic Molecular Dynamics in Small Molecules"*
- 7. Randy Ellingson** (NREL)  
*"TBA"*
- 8. Nikolai Fomin**, E. O. Danilov, A. J. Rodgers, D. L. Snavely (Bowling Green State University)  
*"Nonlinear Optical Properties of Organic Chromophores Immobilized in Sol-Gel Glasses"*
- 9. Rene Gaudoin** (Rutgers University)  
*"A direct approach to excited states in density functional theory"*
- 10. Kirill Igumenshchev** (University of Rochester) and S. Tretiak (LANL) *"Delocalization of photoexcitations in conjugated polymers: a time-dependent density functional theory study"*
- 11. Hose Hodak**, C. Downey, A. Pardi, D. J. Nesbitt (JILA and University of Colorado)  
*"Single Molecule Folding Dynamics of Hammerhead Ribozyme Constructs"*
- 12. Joshua Kennedy**, Z. V. Vardeny (University of Utah), A. Dalton, R. Baughman (UT, Dallas)  
*"A direct approach to excited states in density functional theory"*
- 13. Dmitri Kilin** (University of Washington)  
*"Peak shift modulation for photon echo in molecular dimers"*
- 14. Chaehyuk Ko**, B. Levine, and T. J. Martínez (University of Illinois)  
*"Ab Initio Multiple Spawning Dynamics of the Photoactive Yellow Protein Chromophore"*
- 15. Nadya Kobko** (City University of NY), A. Masunov, S. Tretiak (LANL)  
*"Study of nonlinear optical response in substituted stilbenes with the time-dependent density functional theory"*
- 16. Weinan Leng** and A. Myers Kelley (University of California, Merced)  
*"Resonance Raman study of interchromophore coupling in monomeric and dimeric merocyanine dyes"*
- 17. Sergey Levchenko** and A. I. Krylov (University of Southern California)  
*"Why electronic states of the three dihydroxytoluene isomers are so different? Understanding excited states in open-shell systems by Spin-Flip EOM-CCSD calculations."*
- 18. Alexander Mikhailovsky**, J. Ostrowski, M. Katiyar, and G. Bazan (UCSB)  
*"Control of Radiative Processes Using Surface Plasmon Resonances in Metal Nanostructures"*
- 19. James Murphy**, O. Micic, M. Hanna, R. Ellingson and A. Nozik (NREL and University of Colorado)  
*"Interdot Electronic Coupling in Quantum Dot Arrays observed using Time-Resolved Terahertz Spectroscopy"*



- 20. Hiromi Nakai**, J. Heyd, and G. E. Scuseria (Rice University and Waseda University, Japan)  
*“Theoretical study of the band structure of rutile and anatase titanium dioxide”*
- 21. Ted Ortiz** (University of New Mexico)  
*“TBA”*
- 22. Juan Peralta** and G. E. Scuseria (Rice University)  
*“Relativistic self-consistent field all-electron calculations including the spin-orbit interaction”*
- 23. Andrei Piryatinski**, S. Tretiak, H. Htoon, and V.I. Klimov (LANL) *“Multiparticle Electronic Dynamics in Transition from Zero to One Dimension in Semiconductor Nanostructures”*
- 24. Randy Polson** and Z.V. Vardeny (University of Utah)  
*“Random Lasing from Organic Gain Media”*
- 25. Garry Rumbles** (NREL)  
*“TBA”*
- 26. Karin Schmidt** (University of Arizona) *“Quantum confinement in quasi-one-dimensional solids with strong coupling of Frenkel and Charge Transfer excitons”*
- 27. Eugene Tsiper** (Rutgers University)  
*“Generalized Lanczos method for lowest-frequency excitations in dynamic mean-field calculations”*
- 28. Nina Verdal** and A. Myers Kelley (University of California, Merced)  
*“Coupling of amorphous matrix phonons to the electronic transitions of rigid chromophores”*
- 29. Dmitri Voronine** (Bowling Green State University)  
*“Excited State Dynamics of Mesoscopic Chromophore Aggregates; Dependence on Aggregate Shape”*
- 30. Yongguo Yan** S. Mazumdar, S. Dallakyan, and M. Chandross (University of Arizona)  
*“Designing  $\pi$ -conjugated polymers with light emission in the infrared”*
- 31. Wei Zhuang**, A. Moran, T. Jansen, and Shaul Mukamel (University of Rochester)  
*“Two dimensional vibrational snapshots of peptide relaxation triggered by photoisomerization: MDsimulation”*